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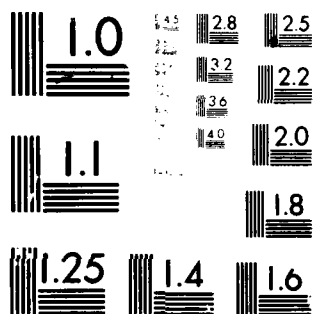
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Aron Kuppermann
Aron Kuppermann
Professor of Chemical Physics

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1. PROJECT ABSTRACT

The purpose of this project was to perform accurate and approximate quantum dynamical calculations on elementary chemical reactions of importance for the fundamental aspects of chemical dynamics and for advanced technologies of interest to the United States Air Force, such as high energy chemical lasers, plume technology, and the chemical effects of high energy radiation. These included calculations of three-atom exchange reactions, breakup collisions, three-body recombinations, vibrational quenching by reaction, tunneling, and electronic branching ratios. The aim of these calculations was to develop an understanding of these processes and to develop benchmark data against which approximate methods may be tested.

2. PROGRESS REPORT

This Final Scientific Report covers a period of two years, from 1 July 1977 through 30 June 1979. During that period, substantial progress was achieved in six areas of endeavor:

- a) Exact quantum calculations of three-dimensional reactive scattering calculations.
- b) The use of symmetrized hyperspherical coordinates in the quantum mechanical study of molecular collisions.
- c) The development of a quantum mechanical method for studying collision-induced dissociation and three-body recombination processes in competition with exchange collisions.
- d) The effect of barrier height on determining the relative vibrational state populations of reaction products.
- e) Effectiveness of chemical reactions as vibrational state deactivators.
- f) Improvements in transition state theory.

In what follows, we describe the work which was performed in each of these six areas.

2.1. Quantum Mechanical Calculations of Three-Dimensional Reactive Scattering Cross Sections.

The prediction and interpretation of the details of chemical reactions from first principles has been a goal of chemistry since the advent of wave mechanics about 50 years ago. However, methodological and computational difficulties have prevented the achievement of this goal until very recently. In 1929, Dirac¹ made his famous statement concerning this matter: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations

much too complicated to be solvable." Insofar as chemical reactions are concerned, only recently have accurate three-dimensional (3D) quantum dynamical calculations on realistic potential energy surfaces for the H_3 system been published.²⁻⁴ These are the only accurate 3D reactive differential cross sections published so far. This development has opened up the possibility of applying the methods developed for the calculations to other systems, and to test the validity of approximate methods. Approximations which turn out to be successful can then be applied to more complex systems for which accurate ab initio calculations cannot presently be performed. This approach to the testing of approximate theories has advantages over the one based on a comparison between theory and experiment. The reason is that potential energy surfaces are not experimentally known. Therefore, it is necessary to make assumptions concerning such surfaces which usually involve some calibration to yield appropriate dynamical behavior. This biases the test of the dynamical model. However, if such a model is used and an accurate quantum dynamical calculation is performed on the same assumed (but fairly realistic) potential energy surface (for electronically adiabatic processes), this logical difficulty disappears and the approximate dynamical model is indeed given a very good test.

During the last two years we have been developing a computer program to apply the general methodology devised previously to 3D triatomic reactions in which two of the three atoms are identical. These processes are of the type $A + BA \rightarrow AB + A$, $A_2 + B$, and their inverse. Triatomic systems of this type that are of interest include the $D + H_2$, $F + H_2$, and $Cl + H_2$ ones. The mathematics of the method have been described in detail elsewhere.³ The computer program in question has been completed and was tested out on the H_3 system. In other words, it was run ignoring the fact that in this example atoms A and B are also identical. The results agreed accurately with those of the previously

developed computer program for systems of the A_3 type, in which the three atoms are identical. This is a very crucial self-consistency check. The A_2B program in question is quite complex, and making it achieve its present state was a major task. In the next year it will be applied initially to the $D + H_2$ reaction where it is expected to yield the first accurate theoretical information on the isotope effect on a chemical reaction.

2.2. Symmetrized Hyperspherical Coordinates for Quantum Mechanical Reactive Scattering. The calculational scheme used in the previous section perceived the dynamics of an ABC triatomic system as being determined by three "half-collisions": $A + BC$, $B + CA$, and $C + AB$. In other words, it examines the behavior of solutions of the Schrödinger equation in each of those three arrangement channel regions. The nature of the reactive process is determined by the requirement that such solutions be smoothly continuous across arbitrarily chosen surfaces in configuration space which separate in a pairwise manner the arrangement channel regions. When the topology of the potential energy surface is such that such pairwise separation surfaces do not exist or have inconvenient shapes, this calculational procedure can become quite cumbersome.

For this reason we have developed a different way of looking at reactive processes, which permits, in addition, the investigation of breakup processes such as $A + BC \rightarrow A + B + C$. This approach is based on symmetrized hyperspherical coordinates⁵ which are defined as follows. Let $\underline{R}'_\alpha, \underline{r}'_\alpha$ be, respectively, the position vector of A with respect to the center of mass of BC and the B-to-C internuclear vector. Similarly, we define $\underline{R}'_\beta, \underline{r}'_\beta$ for B and CA and $\underline{R}'_\gamma, \underline{r}'_\gamma$ for C and AB. These three sets of coordinates can be represented in general by $\underline{R}'_\lambda, \underline{r}'_\lambda$ with $\lambda = \alpha, \beta, \gamma$. It is convenient to replace them by mass-scaled coordinates $\underline{R}_\lambda, \underline{r}_\lambda$ defined by $\underline{R}_\lambda = a_\lambda \underline{R}'_\lambda$ and $\underline{r}_\lambda = a_\lambda^{-1} \underline{r}'_\lambda$, where

$a_\lambda = (\mu_{\lambda, \nu\kappa} / \mu_{\nu\kappa})^{\frac{1}{2}}$, $\mu_{\nu\kappa}$ being the reduced mass of the diatom $A_\nu A_\kappa$, and $\mu_{\lambda, \nu\kappa}$ the reduced mass of the $A_\lambda + A_\nu A_\kappa$ system. A_α , A_β , and A_γ are equivalent to A, B, and C, respectively, and $\lambda\nu\kappa$ is a cyclic permutation of $\alpha\beta\gamma$. In terms of the scaled coordinates, $\underline{R}_\lambda, \underline{r}_\lambda$, the kinetic energy of the system is still diagonal and involves a single λ -independent reduced mass $\mu = [m_A m_B m_C / (m_A + m_B + m_C)]^{\frac{1}{2}}$. The transformation $\underline{R}_\lambda, \underline{r}_\lambda \rightarrow \underline{R}_\nu, \underline{r}_\nu$ is a six-dimensional rigid rotation.

We now define a hyperspherical radius $\rho = (R_\lambda^2 + r_\lambda^2)^{\frac{1}{2}}$ (which turns out to be independent of λ ^{3, 5}) and a symmetrized hyperspherical colatitude angle $\omega_\lambda = 2 \tan^{-1}(r_\lambda / R_\lambda)$ in the 0 to π range. The potential energy for a given electronic state of ABC (under conditions of validity of the Born-Oppenheimer approximation) is a function of the internal coordinates $R_\lambda, r_\lambda, \gamma_\lambda$ (where γ_λ is the angle between \underline{R}_λ and \underline{r}_λ in the 0 to π range) or, equivalently, of the symmetrized hyperspherical coordinates $\rho, \omega_\lambda, \gamma_\lambda$ which constitute a different kind of internal coordinates. If we consider the latter as the spherical polar coordinates of a point in a three-dimensional configuration space $OX_\lambda Y_\lambda Z_\lambda$, there exists a one-to-one correspondence between the half space $Y_\lambda \geq 0$ and geometrical configurations of the ABC system. Furthermore, a change from $\rho, \omega_\lambda, \gamma_\lambda$ to $\rho, \omega_\nu, \gamma_\nu$ corresponds to a rigid rotation around OY_λ in this space. This means that equipotential surfaces in it do not change shape upon a $\lambda \rightarrow \nu$ coordinate transformation. These properties constitute the basis for our new reactive scattering approach. In addition to $\rho, \omega_\lambda, \gamma_\lambda$, let us consider the polar angles $\theta_\lambda, \phi_\lambda$ of \underline{R}_λ with respect to laboratory-fixed axes and a tumbling angle ψ_λ of the instantaneous ABC plane around \underline{R}_λ . These six variables are very appropriate for expressing and solving the reactive scattering problem.⁶

We first expand the solutions $\Psi(\underline{R}_\lambda, \underline{r}_\lambda)$ of the corresponding Schrödinger equation in partial waves $\Psi^{JM}(\underline{R}_\lambda, \underline{r}_\lambda)$ which are simultaneous eigenfunctions of the hamiltonian, of the square of the total angular momentum, and of its

laboratory z-axis component with eigenvalues $E, J(J+1)\hbar^2$, and $M\hbar$, respectively. These eigenfunctions are in turn expanded as

$$\Psi^{JM}(\underline{R}_\lambda, \underline{r}_\lambda) = \sum_{\Omega_\lambda=-J}^J D_{M\Omega_\lambda}^J(\varphi_\lambda, \theta_\lambda, \psi_\lambda) \Psi_{\Omega_\lambda}^J(\rho, \omega_\lambda, \gamma_\lambda),$$

where the $D_{M\Omega_\lambda}^J$ are the elements of the Wigner rotation matrix. The six-dimensional Schrödinger equation can then be replaced by the following set of coupled partial differential equations in the three symmetrized hyperspherical coordinates $\rho, \omega_\lambda, \gamma_\lambda$:

$$H_{\Omega_\lambda, \Omega_\lambda-1}^J \Psi_{\Omega_\lambda-1}^J + H_{\Omega_\lambda, \Omega_\lambda}^J \Psi_{\Omega_\lambda}^J + H_{\Omega_\lambda, \Omega_\lambda+1}^J \Psi_{\Omega_\lambda+1}^J = E \Psi_{\Omega_\lambda}^J$$

$$\Omega_\lambda = -J, -J+1, \dots, J.$$

The operator $H_{\Omega_\lambda, \Omega_\lambda}^J$ contains the potential energy function $V(\rho, \omega_\lambda, \gamma_\lambda)$, whereas $H_{\Omega_\lambda, \Omega_\lambda \pm 1}^J$ contain only angular momentum coupling terms.³ The important characteristic which distinguishes reactive from nonreactive systems is that in the former V has regions of accessibility corresponding to more than one arrangement channel. If all three molecules, AB, BC, and CA, are stable, there are three arrangement channels to be considered. For example, for the H_3 system, V is represented in Figure 1 for the Porter-Karplus surface.⁵ Part a of that figure depicts the collinear arrangements and part b those in which \underline{R}_α is perpendicular to \underline{r}_α . As can be seen, the three arrangement channel tubular regions are interconnected by passageways whose cross section is represented in the lower part of Figure 1b. If the system were nonreactive, as the ground electronic state of HeH_2 , there would be only one tubular region, corresponding to the $He + H_2$ arrangement channel. Collisions in reactive systems permit flux from one arrangement channel to be directed into the

FIGURE 1.

Equipotential surfaces for H_3 . The cartesian coordinates $X_\alpha, Y_\alpha, Z_\alpha$ are $\rho \sin \theta_\alpha \cos \gamma_\alpha$, $\rho \sin \theta_\alpha \sin \gamma_\alpha$, and $\rho \cos \theta_\alpha$, respectively. The range of γ_α was extended from $(0, \pi)$ to $(-\pi, \pi)$ by setting, for $\gamma_\alpha < 0$, $V(\rho, \theta_\alpha, -\gamma_\alpha) = V(\rho, \theta_\alpha, \gamma_\alpha)$. The curves are intersections of $V(\rho, \theta_\alpha, \gamma_\alpha) = E$ surfaces with the perpendicular planes $OX_\alpha Z_\alpha$ (Figure 1a) and $OY_\alpha Z_\alpha$ (Figure 1b). The origin of measurement of E is the minimum of the diatomic potential energy curve with the third atom removed. The values of E range from 0.3 eV to 1.5 eV in steps of 0.3 eV, as indicated on top of the figure. All points on Figure 1a and those on the OZ_α axis of Figure 1b correspond to collinear configurations. All other points on Figure 1b correspond to configurations in which \hat{R}_α is perpendicular to \hat{r}_α . The OZ_λ axes ($\lambda = \alpha, \beta, \gamma$) in Figure 1a, as $\rho \rightarrow \infty$, correspond to the three separated atom-diatom arrangements. The bottom part of Figure 1b corresponds to the region halfway between configurations $A_\gamma + A_\alpha A_\beta$ and $A_\gamma A_\alpha + A_\beta$. All classically allowed pathways leading from one to the other of these configurations, at total energies not exceeding 0.6 eV, must pass through the hatched area enclosed by the corresponding equipotential.

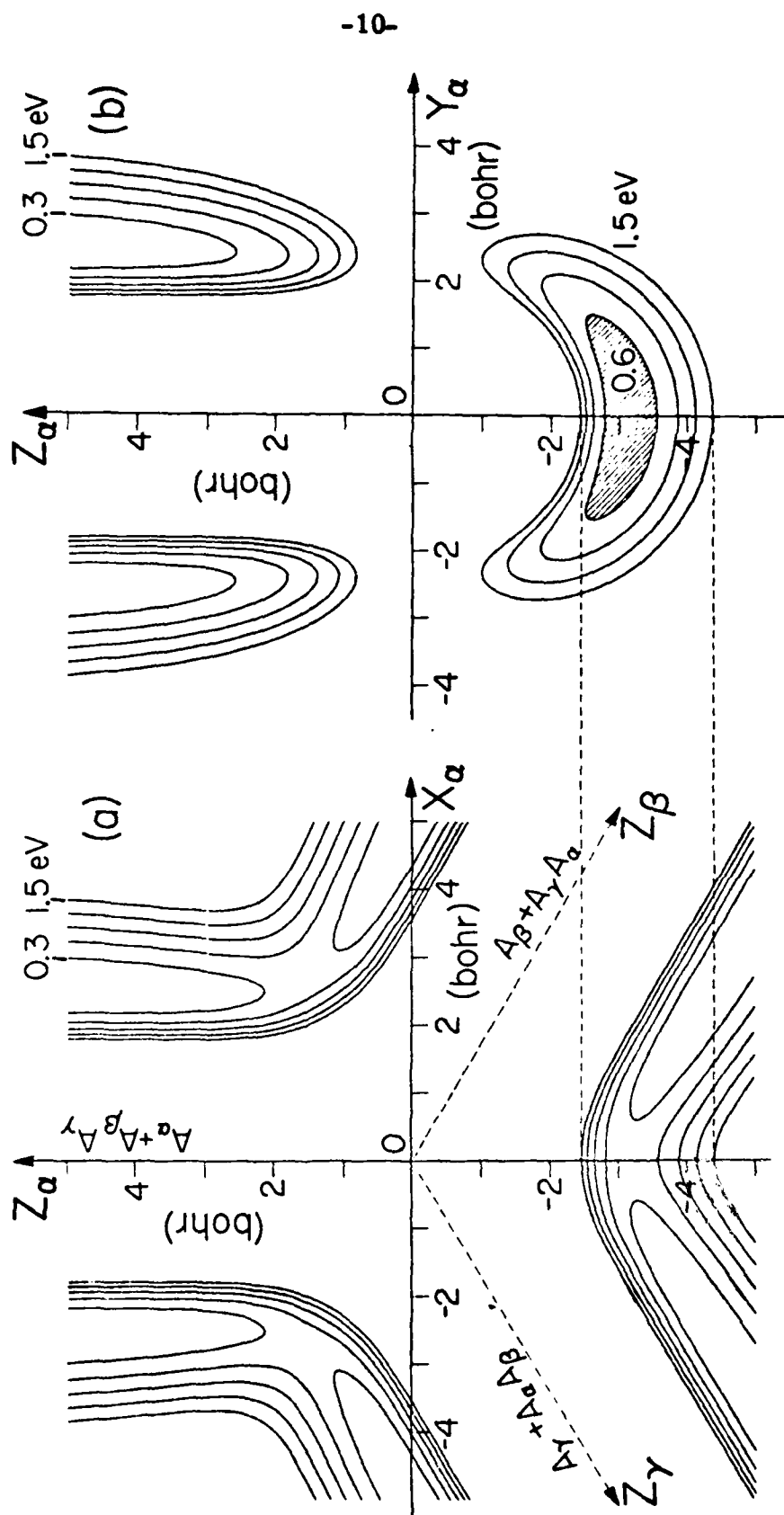


Figure 1

others, and it is this which makes reactive scattering differ from nonreactive and complicates the pursuit of solutions to Eq.(1). As described above, the change of coordinates $\rho, \omega_\lambda, \gamma_\lambda \rightarrow \rho, \omega_\nu, \gamma_\nu$ merely rotates equipotential surfaces of V around OY_λ without distorting them. It is this property which is the basis of the method to solve the reactive scattering problems we are describing. The main hamiltonian operator $H_{\Omega_\lambda, \Omega_\lambda}^J(\rho, \omega_\lambda, \gamma_\lambda)$, in addition to containing V , has kinetic energy terms, part of which closely resemble the angular kinetic energy of a particle of mass μ (defined at the beginning of this section) moving in a three-dimensional physical space. This suggests that we define a reference hamiltonian $H_0(\bar{\rho}, \omega_\lambda, \gamma_\lambda)$, containing V , with ω_λ and γ_λ as variables and $\bar{\rho}$ as a fixed parameter. In other words, H_0 is the hamiltonian of a particle of mass μ constrained to move on a spherical surface of radius $\bar{\rho}$ and subject to the potential $V(\bar{\rho}, \omega_\lambda, \gamma_\lambda)$. The eigenfunctions of H_0 , which we call surface functions, sample $V(\bar{\rho}, \omega_\lambda, \gamma_\lambda)$ in the regions of all three arrangement channels, and form a convenient complete discrete set in terms of which we may expand the $\Psi_{\Omega_\lambda}^J(\rho, \omega_\lambda, \gamma_\lambda)$. This set furthermore samples the positions of configuration space outside of the atom-diatom arrangement channel regions and therefore provides a discrete representation of the dissociation continuum $A + B + C$,⁶ which is suitable for the investigation of breakup collisions and three-body recombinations. Performing the expansion just mentioned for regions of configuration space in which A , B , and C strongly interact with each other, we obtain a set of coupled radial equations in variable ρ . We integrate these starting from a sufficiently small value of ρ such that $\Psi_{\Omega_\lambda}^J$ can be assumed to vanish, and switch surface functions (i.e., increase the value of $\bar{\rho}$) as needed to maintain the goodness of the expansion with the smallest possible number of basis functions. This integration is continued until ρ reaches regions of configuration space in which arrangements α , β , and γ have stopped interacting

with each other. We then integrate separately the coupled equations in each of the three separate arrangement channels into their asymptotic regions using as basis functions the eigenfunctions of BC, CA, and AB, respectively, as is done in nonreactive scattering. The scattering matrix \hat{S}_J is obtained from the asymptotic behavior of the wavefunction. The same method could be used for scattering in nonreactive systems if desired. The hyperspherical radius ρ is a natural "propagation" variable for both reactive and nonreactive systems, and $\omega_\lambda, \gamma_\lambda$ sample all arrangement channel regions simultaneously (i.e., without having to switch from λ coordinates to ν coordinates). In other words, the λ surface functions sample the ν arrangement channel region as well as the λ arrangement channel region.

We have over the past two years been developing the computer programs which implement the methodology described above. The program for integrating the coupled Schrödinger equations from small values of ρ , for which the wavefunction vanishes (since V is very large), through the strong (saddle-point) interaction region, to the region where the three arrangement channels $A + BC$, $AB + C$, and $AC + B$ no longer interact with one another, has also been written and checked out. At the corresponding range of ρ , a change is made from symmetrized hyperspherical coordinates to cartesian ones, with the help of a "projection" program, which has also been written and checked out. The integration of the Schrödinger equations between the projection region and the asymptotic region of configuration space (in which A no longer interacts with BC , nor B with AC , or C with AB) is performed by another program, which has also been written and checked out. The last step in this overall procedure is a reactance matrix analysis. The program for performing it has been written, and is currently being tested. All of these programs (except the one which calculates the basis functions) have been written initially for the total angular momentum quantum

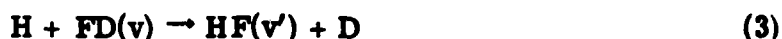
number $J = 0$. After the reactance matrix test is complete, they will be extended to $J \neq 0$ and test calculations will be made for the $H + H_2$ system, for which independent results are available for comparison purposes. The indications we have so far are that this will be a very efficient new method, significantly faster than our present one.²⁻⁴ It may permit reactive scattering calculations to be performed for more complex systems. In addition, the symmetrized hyperspherical coordinate approach lends itself to the development of novel approximate reaction dynamic theories, significantly different from those based on cartesian coordinates. Such approximations will be considered in the future.

2.3. Collision-Induced Dissociation and Three-Body Recombination Processes.

No accurate quantum calculations of the type $A + BC \rightarrow A + B + C$ or its reverse have been performed so far, and as a result no firm information exists on the magnitude of quantum effects on collision-induced molecular dissociation or three-atom recombination elementary processes. The difficulty is a conceptual one. The $A + B + C$ channel involves two continua, and methods for handling them are not known. Some time ago, Delves⁶ showed how one could use hyperspherical coordinates to reduce this problem to one involving only one continuum, that associated with the hyperradius. We have used these variables to develop a method for studying the $A + BC$ collinear system, and applied it to the $H + H_2 \rightarrow H_2 + H$ reaction over the relative energy range 0 to 1.5 eV. The dissociation channel, which opens up at about 4.5 eV, is closed at those energies. The results agreed quite well with those of previous calculations.⁷ These calculations are currently being extended to higher energies, at which the effect of closed dissociative channels will start having an influence, and for which other methods are no longer adequate. Subsequently, they will be used at energies beyond the H_2 dissociation energy. Once these collinear quantum collision-induced

dissociation and three-body recombination results are in hand, corresponding quasi-classical calculations will be performed to determine the magnitude of quantum effects in this system.

2.4. Effects of Barrier Height on Vibrational Branching Ratios. It has been suggested previously⁸ that the exchange reactions



may play an important role in the vibrational deactivation ($\nu' < \nu$) of vibrationally excited HF or DF molecules in the fluorine-hydrogen chemical lasers. The performance of cw fluorine-hydrogen lasers suggests that the $\nu = 4, 5, 6$ levels of HF are more effectively quenched than the $\nu = 2, 3$ by a mechanism not well understood. Ab initio calculations⁹ of the barrier height for this reaction have indicated that it may be of the order of 30 or 40 kcal/mole, much higher than previously assumed. This led to the working hypothesis that the reactions (1) through (3) above are effective for vibrational energies greater than the barrier height E_b but are ineffective for energies smaller than E_b . We have previously performed an extensive series of quantum dynamical calculations for a collinear model of these reactions using values of E_b of 1.5, 5, 10, 20, 30, and 40 kcal/mole. The energy range over which these calculations were performed permitted the study of reactions (1) and (3) for $\nu = 0$ through 6, and of reaction (2) for $\nu = 0$ through 5. Over the last year we used the resulting reaction probabilities to calculate rate constants for reactions (1) and (2). The results indicate that although the $\nu = 3$ state of HF has a vibrational energy of approximately 38 kcal/mole (measured with respect to the bottom of the HF well), the fraction f of the deactivation rate constant which is due to the

exchange reaction decreases (at 300°K) from 77% for $E_b = 1.5$ kcal/mole to below 5% for $E_b > 20$ kcal. For $v = 5$, the vibrational energy is approximately 57 kcal/mole, and f at 300°K drops from 75% for $E_b = 1.5$ kcal/mole to below 10% for $E_b > 30$ kcal/mole. The activation energy for reaction (1), for a given v to all products with $v' < v$, around 300°K, is 0.9 kcal/mole for $v = 3$ and 4 and 0.7 kcal/mole for $v = 5$, all for $E_b = 1.5$ kcal/mole. The corresponding energies for the nonreactive process are 1.1, 1.0, and 0.9 kcal/mole, respectively. This insensitivity with respect to v of the activation energies for the reactive and nonreactive deactivation processes in the temperature region around 300°K persists as the barrier height increases. For $E_b = 40$ kcal/mole, the $v = 3, 4$, and 5 activation energies for deactivation by exchange are 1.9, 1.5, and 0.9 kcal/mole, and for deactivation without exchange are 0.3, 1.0, and 1.4 kcal/mole, respectively. The conclusion to be derived from this entire set of calculations is that for barrier heights of 20 kcal or greater, vibrational deactivation by the exchange reactions of HF with H atoms (in a collinear model) is not an important mechanism, and cannot account for the more effective quenching of the $v = 4, 5$, or 6 levels of HF with respect to the $v = 2, 3$ ones mentioned above.

For reaction (2), room temperature activation energies for $0-0$, $0-1$, $0-2$, and $0-3$ reactive processes were calculated. They are approximately equal to the endothermicity ΔE of the process and independent of E_b for values of E_b smaller than ΔE ; for values of $E_b > \Delta E$, they become approximately independent of v' and equal to about 80% of E_b . The deactivation rate constants for this reaction are presently being analyzed.

2.5. Relative Effectiveness of the $H + HF(v) \rightarrow H + HF(v')$, $H_2(v'') + F$ Processes as Deactivators of Vibrationally Excited HF. Since the reaction $F + H_2 (v = 0) \rightarrow FH(v') + H$ produces, at room temperature, mainly products with $v' = 2, 3$, it is interesting to examine the relative probabilities of the $H + FH(v) \rightarrow H + FH(v' < v)$ and $H + FH(v) \rightarrow H_2 + F$ processes as a function of v , to test the relative effectiveness of the abstraction reaction as a deactivator of vibrationally excited FH molecules by collision with H atoms. We have performed such calculations for a collinear quantum mechanical model of this system. At 300°K we found that the fractional deactivation by reaction decreased from 86% for $v = 3$ to 40% for $v = 5$. This decrease was due principally to a decrease of the reaction rate constant with increasing v . In addition, the total reactive plus nonreactive deactivation by collision rate constant decreases by a factor of over 10 in comparing the 300°K $v = 3$ value with the corresponding $v = 5$ one. The conclusion is that this process, insofar as this collinear model is concerned, also does not lead to a more effective deactivation of $v = 3$ FH molecules vis-a-vis $v > 3$ ones.

2.6. Improvements of Transition State Theory. We have developed and published an exact transition state theory (TST).¹⁰ Calculations were performed using the coplanar reaction transmission coefficient κ to obtain improved TST rate constants for the $H + H_2$ (para) $\rightarrow H_2$ (ortho) + H rate constants. At 200°K, using the exact collinear (i. e., two-mathematical dimensional-2 MD) κ , the TST rate constant was smaller than the correct one by a factor of 9. Using the coplanar κ (obtained from 4 MD accurate scattering calculations^{11,12}), the TST rate constant was still off by a factor of 3.2 at this temperature and of 1.6 at 300°K. This indicates that if one wishes to have a rate constant theory good to 10% or 20% at room temperature for highly quantum systems having activation

barriers of the order of 10 kcal/mole, the theory must contain essentially all of the collision dynamics. Even a coplanar approximation, for a triatomic case, which samples the entire potential energy function but omits the coupling of tumbling motions with in-plane motions, introduces this unexpectedly large error of 60% at room temperature for the para - ortho hydrogen atom plus hydrogen molecule exchange reaction rate constant. This is a rather disappointing state of affairs which will require the development of better approximate reaction dynamic theories than those presently available.

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3. SUMMARY OF PROGRESS

In summary, the following progress was achieved over the two years for which this grant was awarded:

- a) A complex computer program for doing accurate three-dimensional quantum mechanical reactive scattering calculations on triatomic systems of the type A_2B was developed.
- b) Another program for doing similar calculations on A_3 systems using symmetrized hyperspherical coordinates was developed.
- c) Collinear triatom reactive calculations using hyperspherical coordinates were performed and gave results in agreement with previous methods for energies up to one-third of the dissociation energy.
- d) The effect of barrier height on the outcome of the collinear reaction $H + FH(v) \rightarrow HF(v') + H$ and some of its isotopic counterparts was investigated in detail. The conclusion was that this exchange reaction is not an efficient mechanism for deactivation of $FH(v)$ for barrier heights of the order of 30 kcal/mole or greater.
- e) It was found that for collinear collisions $H + HF(v)$, the abstraction reaction to give $H_2 + F$ accounts for a substantial fraction of the deactivation rate constants at room temperature. However, the $v = 3$ FH molecules are not deactivated by the process more effectively than the $v > 3$ ones, in contradiction with previous suggestions.
- f) An exact version of transition state theory was developed that establishes the correspondence between this theory and the collisions theory of bimolecular reactions.

4. PUBLICATIONS

1. An Exact Quantum Mechanical Transition State Theory. 1. An Overview.
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2. Comment on "Theory of Collisions Between an Atom and a Diatomic Molecule in the Body-Fixed Coordinate System."
G. C. Schatz and A. Kuppermann.
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3. Vibrational Deactivation on Chemically Reactive Potential Surfaces: An Exact Quantum Study of a Low Barrier Collinear Model of $H + FH$, $D + FD$, $H + FD$, and $D + FH$.
G. C. Schatz and A. Kuppermann.
J. Chem. Phys., in press.
4. Theoretical Aspects of the Mechanism of Simple Chemical Reactions.
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